Exact Dirac equation calculation of ionization and pair production induced by ultrarelativistic heavy ions

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Abstract

An exact solution of the time-dependent Dirac equation for ionization and pair production induced by ultrarelativistic heavy ion collisions is presented. Exact transition probabilities, equivalent to those that would be obtained in an untruncated basis coupled channels calculation, are presented. Exact bound-electron positron pair production probabilities are calculated to be mostly smaller than those calculated with the same potential in perturbation theory at impact parameters small enough for differences to occur.

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The calculation of bound-electron positron pair production induced by relativisitic heavy ion collisions has been a subject great interest recently [1]. One motivation for this interest is the anticipated large rates of pair production with an electron captured into a bound state of one of the pair of fully stripped ions in a collider such as the Brookhaven Relativistic Heavy-Ion Collider (RHIC) or the CERN Large Hadron Collider (LHC). The capture process will provide an important limit on the beam lifetime since change of the charge of an ion leads to the loss of that ion from the beam. Early non-perturbative coupled channel calculations showed an enhancement of some two orders of magnitude [2] over corresponding perturbation theory calculations at small impact parameters for Pb + Pb reactions at relatively low relativistivc energies (e.g., γ=2.3). These results motivated an extensive investigation at ultrarelativistic energies such as will occur at RHIC (γ=23 000), and the problem of non-

perturbative enhancemant was shown to present no serious obstacle to machine performance. It was found that the enhancement over perturbation theory systematically decreased with increasing basis size of the coupled channels calculations up to the largest basis size attainable, where the total non-perturbative enhancement was found to be only of order 10% of the total cross section [3]. It was further observed that the limited enhancement over perturbation theory applied as well at other ultrarelativistic energies (such as at LHC) since the probabilities at impact parameters small enough to have non-perturbative effects are γ independent at large γ [4].

In this Letter it will be shown that, in the ultrarelativistic limit, the time-dependent Dirac equation can be solved exactly, and one discovers that exact semi-classical probabilities of bound-electron positron pair production are actually less than those calculated in perturbation theory. One also obtains exact results for single electron ionization and finds that they are consistent with unitarity. As a corollary, ionization calculations can now be carried out without consideration of the continuum final states but rather by considering the flux lost from the initial bound state.

It has recently been shown [5] that, in the appropriate gauge [4], the Coulomb potential produced by an ultrarelativistic particle (such as a heavy ion) in uniform motion takes the following form

$$V(\boldsymbol{\rho}, z, t) = -\delta(z - t)\alpha Z_P(1 - \alpha_z) \ln \frac{(\mathbf{b} - \boldsymbol{\rho})^2}{b^2}. \tag{1}$$

$\mathbf{b}$ is the impact parameter, perpendicular to the z–axis along which the ion travels, $\boldsymbol{\rho}$, z, and t are the coordinates of the potential relative to a fixed target (or ion), α_z is the Dirac matrix, α is the fine structure constant, and Z_P, v and γ are the charge, velocity and γ factor the moving ion ($\gamma = 1/\sqrt{1 - v^2}$). This is the physically relevant ultrarelativistic potential since it was obtained by ignoring terms in $1/\gamma^2$ [5] [4]. The b^2 in the denominator of the logarithm is removable by a gauge transformation, and if one wished to have a potential with the same gauge for all impact parameters one would remove it. However, the freedom to include or remove the extra b^2 will be retained for possible computational convenience

and as a minimal test of gauge invariance.

It was suggested in Ref. [5] that the reduction of the interaction from three dimensions to the two of Eq.(1) might make direct solution of the time-dependent Dirac equation, without using coupled channels, a viable alternative for the calculations of pair production induced by ultrarelativistic heavy ions. I point out in this Letter that, in fact, the delta function form of Eq.(1) allows exact evaluation of the transition amplitudes for pair production without using coupled channels. The form that the amplitudes take is that of perturbation theory, but with a universal effective interaction, modified from the the lowest order interaction to exactly include coupling to all orders.

The time-dependent Dirac equation that I wish to solve is

$$\begin{aligned}\frac{i\partial\Psi(\mathbf{r},t)}{\partial t} &= \Big[H_1\Big]\Psi(\mathbf{r},t)\\ &= \Big[H_0 - V(\boldsymbol{\rho},z,t)\Big]\Psi(\mathbf{r},t)\\ &= \Big[H_0 + \delta(z-t)\alpha Z_P(1-\alpha_z)\\ &\qquad \times \ln\left(\mathbf{b}-\boldsymbol{\rho}\right)^2\Big]\Psi(\mathbf{r},t),\end{aligned} \tag{2}$$

where H_0 is a time-independent Dirac hamiltonian, in this case of an electron in the Coulomb field of a one of the ions (target) in its rest frame,

$$H_0 = \boldsymbol{\alpha}\mathbf{p} + \beta - \alpha Z_T/r, \tag{3}$$

$\Psi(\mathbf{r},t)$ is the exact four component time-dependent Dirac spinor solution, and for typographical simplicity the gauge explicitly shown is without the b^2 in the denominator of the logarithm.

In the usual coupled channels approach [2] one expands the solutions of Eq.(2) in a time-independent basis of eigenfunctions of H_0,

$$\Psi^j(\mathbf{r},t) = \sum_k a_k^j(t)\phi_k(r)e^{-iE_kt}, \tag{4}$$

and then substitutes Eq.(4) into both left and right hand sides of Eq.(2) to obtain coupled equations for the time-dependent amplitudes, $a_k^j(t)$. For electron-positron pair production ϕ_k

includes bound electron states, continuum electron states, and states in the negative energy continuum. Pair production may be represented as a transition from an initial negative continuum state to a final bound or positive continuum electron state. How this scheme preserves the Pauli principle for non-interacting electrons and how time reversal can be exploited in these calculations has been previously discussed. [2]

The present treatment differs from the usual coupled channels approach in that I substitute Eq.(4) only into the left hand side of Eq.(2). In the usual way, I then multiply both sides by any particular state ϕ_f, and perform the spatial integration to obtain

$$\frac{da_f^j(t)}{dt} = -ie^{iE_f t}\langle\phi_f|\delta(z-t)\alpha Z_P(1-\alpha_z) \times \ln(\mathbf{b}-\boldsymbol{\rho})^2|\Psi^j(\mathbf{r},t)\rangle. \tag{5}$$

The initial condition, $a_f^j(t=-\infty)=\delta_{fj}$, is specified by the index j and given equivalently

$$\Psi^j(\mathbf{r},t=-\infty)=\phi_j(r)e^{-iE_j t_{-\infty}}. \tag{6}$$

Of course, if one knew the exact solution, $\Psi^j(\mathbf{r},t)$, then it would be possible simply to integrate Eq.(5) over t and obtain the exact scattering amplitudes, $a_f^j(t=\infty)$. But the delta function and $(1-\alpha_z)$ factor in Eq.(5) mean that one needs only to know $(1-\alpha_z)\Psi^j(\mathbf{r},t)$ at $z=t$. And it turns out that one can obtain $(1-\alpha_z)$ times the exact solution of Eq.(2) in the region near $z=t$ in the following way. First temporarily express Eq.(2) in terms of the usual light cone coordinates

$$x^+ = \frac{1}{\sqrt{2}}(t+z)$$
$$x^- = \frac{1}{\sqrt{2}}(t-z) \tag{7}$$

instead of t and z. Integration of x^- across the δ function then gives

$$(1-\alpha_z)\Psi^j(\mathbf{r},t)=(1-\alpha_z)e^{-i\theta(t-z)\alpha Z_P\ln(\mathbf{b}-\boldsymbol{\rho})^2}\phi_j(r)e^{-iE_j t}, \tag{8}$$

valid for $t<z$ and in the region near $t=z$ (i.e at $t=z$ and $t=z+\epsilon$). Substituting Eq.(8) into Eq.(5) and integrating over t, I obtain

$$a_f^j(t=\infty) = \delta_{fj} - i\int_{-\infty}^{\infty} dt e^{i(E_f-E_j)t} \times \langle\phi_f|\delta(z-t)\alpha Z_P(1-\alpha_z)\ln(\mathbf{b}-\boldsymbol{\rho})^2 \times|e^{-i\theta(t-z)\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2}\phi_j\rangle. \quad (9)$$

Now since by definition, $\delta(u) = d\theta(u)/du$, one obtains upon carrying out the t integration

$$a_f^j(t=\infty) = \delta_{fj} + \langle\phi_f|(1-\alpha_z)e^{i(E_f-E_j)z} \times(e^{-i\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1)|\phi_j\rangle. \quad (10)$$

thus Eq.(9) may be equivalently expressed in the form

$$a_f^j(t=\infty) = \delta_{fj} + \int_{-\infty}^{\infty} dt e^{i(E_f-E_j)t}\langle\phi_f|\delta(z-t)(1-\alpha_z) \times(e^{-i\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1)|\phi_j\rangle \quad (11)$$

since Eq.(10) trivially follows from it. We make use of Eq.(11) for the calculations since the angular momentum algebra of the computer code makes use of the Legendre polynomial series for the δ function [5] [4].

One now has a simple matrix element expression that is equivalent to the solution of the full coupled channels problem with no truncation of basis. The full solution of the problem, Eq.(11), is in perturbation theory form, but with a universal effective interaction $i\delta(z-t)(1-\alpha_z)(e^{-i\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1)$ instead of the perturbation interaction $\delta(z-t)(1-\alpha_z)\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2$. The only difference between the perturbative and exact matrix element expressions comes in the m-dependent form factors of the interaction, where instead of the analytical Fourier transforms [5] [4] of the real $\ln(\mathbf{b}-\boldsymbol{\rho})^2$ one must substitute Fourier transforms of the complex $i(e^{-i\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1)/\alpha Z_P$ to be evaluated numerically. These exact matrix elements exhibit time reversal symmetry because they are in perturbation theory form with an effective potential.

In the conventional coupled channels method of calculating bound-electron positron pair production one makes use of time reversal and makes the bound electron the initial state [2]. Both positive and negative electron states are coupled. Since the rate of excitation

to negative continuum states is about three orders of magnitude smaller than to positive excited electron states, one thereby also calculates the ionization probability for a single bound electron. From Eq.(10) one may obtain in simple form the exact survival probability of an initial state j

$$P_j(b) = |\langle\phi_j|(1-\alpha_z)e^{-i\alpha Z_P \ln(\mathbf{b}-\boldsymbol{\rho})^2}|\phi_j\rangle|^2. \tag{12}$$

In our previously reported large basis coupled channels calculations of bound-electron positron pair production [3] we found about an overall non-perturbative enhancement of 7 ± 2 barns over the 112 barn perturbation theory result for Pb + Pb at RHIC [6]. For large contributing impact parameters we found a negligible non-perturbative enhancement. For the smallest impact parameters our best truncated calculations showed non-perturbative enhancement still on the order of a factor of two. Parallel calculations have now been carried out using the present exact expressions. Results are presented in Table I. At every impact parameter (except zero) the exact probability is smaller than the perturbation theory result. Contrary to our previous result, the exact formalism yield a small suppression rather than enhancement for the rate of bound-electron positron pair production due to non-perturbative effects. For a large set of final states (corresponding to 61% of the perturbation theory cross section) I find the exact evaluation yields a cross section about 3 barns *less* than the perturbation theory evaluation. The corresponding coupled channels calculation gave about 9 barns *more* than perturbation theory.

A calculation of exact amplitudes for excitation of an initial electron state into allowed final states should exhibit unitarity, which, of course, is absent in perturbation theory. To demonstrate that there is no apparent violation of unitarity, calculations of single electron ionization have been performed at various impact parameters. Results are shown in Table II. Because of the huge low excitation energy contribution to ionization, the cuttoff at $|k| \leq 7$ and $\mathrm{E} \leq 16.8 m_e c^2$ apparently covers a relatively greater part of the ionization cross section (about 90%) than the bound-electron positron cross section (61%). Note that at no impact parameter does the sum of final state bound and continuum probabilities exceed unity; the

10% of the continuum electron probability missing is presumably due to the cuttoff in energy and angular momentum, and is not inconsistent with a smooth extrapolation of $|k|$ and E to infinity. To look at it another way, note that with the present method single electron ionization cross sections can be can be calculated without even considering continuum wave functions. One simply subtracts the sum of the ground state survival probability (column 2) and the excited bound state probabilities (column 3) from unity at each impact parameter to obtain the ionization probability at that impact parameter.

One might reasonably ask what is the physical reason that the exact probablilities are less than those calculated in perturbation theory. For the ionization calculations the answer is clearly unitarity: in the limit of large αZ_P the sum of all perturbative probabilities for transitions to excited states must eventually exceed unity. An exact calculation must maintain conservation of probability. And although the sum of the perturbative bound-electron positron probabilities is several orders of magnitude smaller, it too must violate unitarity in the strong coupling limit.

But there is another aspect of the reaction that explains the failure of coupled channels to provide the correct sign of the correction to perturbation theory for bound-electron positron production: the reaction is highly adiabatic. Figure 1 shows the time development of the total flux in ground state electron plus continuum positron states for a relatively small atomic impact parameter (125 fm) where the time dependent field is relatively strong. The time-dependent component of the field adiabatically excites and then deexcites bound-electron positron pairs. There is a very delicate cancellation in the positive and negative time contributions to the amplitudes. The exact probability (solid line) rises and falls similarly with the perturbative probability (dashed line) but with a smaller magnitude. The coupled channels calculation (dot-dashed line) has the smallest maximum of the curves (at $t = 0$), but is the largest asymptotically. The coupled channels calculation was performed using rather crude wave packets for the unbound negative and positive electrons [3]. The exact and perturbative calculations were performed using continuum wave functions (heavy lines) with the same calculations performed using corresponding wave packets shown in the

faint lines for comparison.

In a simple test of gauge invariance the exact calculation using continuum wave functions apparently passes, but the corresponding calculation using wave packets is less successful. Because the analytical Fourier series of the perturbative potential arises from the gauge of Eq.(1), that gauge has been utilized in the calculations so far reported here (except, of course, at $b = 0$). Thus to remove the b^2 in the denominator of the logarithm, one must add a corresponding scalar $\ln b^2$ term to the interaction. At large b the dominant term of the Fourier series is of dipole form, ρ/b, leading to the $1/b^2$ falloff of the probabilities. But the $\ln b^2$ term added by the gauge transformation increases with b while the physical dipole term decreases. Calculations have therefore been performed at $b = 8000$ fm to test gauge invariance. With continuum wave functions the exact result shows a change from 1.036×10^{-6} to 1.062×10^{-6} under the gauge tranformation while the corresponding wave packet results goes from 1.041×10^{-6} to 1.244×10^{-6}. These results were calculated at a mesh size of .025 with the differences in the two gauges dropping precipitously from those calculated at our standard mesh of .05 in the continuum case but not in the wave packet case. There is no surprise here. We would not expect calculations done with wave packets to be exactly gauge invariant. The packet states are not exact eigenfunctions of the time-independent hamiltonian H_0 and there is a lack completeness. On the other hand, using continuum wave functions, no disagreements inconsitent with expected numerical accuracy were found between exploratory gauge transformed calculations and the results of Tables I and II. For example, in the strong coupling impact parameter case of $b = 125$ fm the ionization probability changes by 0.2% under the gauge transformation and the bound-electron positron probability changes by 0.8% under the same transformation.

Apparently some combination of basis truncation and the necessity of using wave packets for continuum-continuum coupling provides an intractable limitation on the coupled channels method, thereby making it incapable of adequate evaluation of the adiabatic cancellation. This failure of the coupled channels method in the ultrarelativistic limit makes one question its utility even at more modest relativisitic energies, where the same properties

of adiabaticity, basis truncation, and wave packets remain.

The above exact method should have other applications in the future. The corresponding perturbation theory cross section for continuum-electron positron pair production at RHIC is about 30,000 barns. Non-perturbative calculations for this process have so far been prohibitive in difficulty because of the large number of energy and angular momentum states that are coupled. The present approach now seems to make the problem tractable. It allows the exact cross section to be calculated for any particular electron-positron pair in an expression decoupled from all the other pairs.

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FIGURES

FIG. 1. Probability of excitation of a K-orbit electron plus any continuum positron by a Pb ion impinging on a Pb ion target. Impact parameter is 125 fm. Time is in natural units (386 fm.)

TABLES

TABLE I. Bound-electron positron pair production probabilities for Pb + Pb (to be multiplied by 2×10^{-6}) are in the second and third columns. The fourth and fifth columns are in barns and represent the cross section differences from perturbation theory in the annulus from $b/\sqrt{2}$ to $\sqrt{2}b$.

b(fm)	Exact	Perturb.	Exact Enhance.	C. C. Enhance.
0	289.	283.	.001	$< .08$
62.5	271.	505.	$-.08$	$< .22$
125	330.	487.	$-.21$	.53
250	297.	432.	$-.73$	.73
500	171.	216.	$-.98$	1.26
1000	61.5	67.7	$-.54$	3.00
2000	16.57	16.92	$-.12$	2.30
4000	4.144	4.160	$-.02$	.82
8000	1.0348	1.0357	$-.005$	.20

TABLE II. Ionization and Unitarity: Probabilities for Pb + Pb

b(fm)	e^-_{gr}	$\sum_{bnd} e^-_{ex}$	$\sum_{cont} e^-$	$\sum e^-$
0	.428	.100	.457	.985
31.25	.430	.099	.454	.983
62.5	.434	.099	.444	.978
125	.447	.101	.426	.974
250	.488	.104	.381	.974
500	.582	.101	.292	.975
1000	.730	.086	.169	.986
2000	.890	.054	.052	.996
4000	.971	.019	.009	.999
8000	.9927	.0051	.0020	.9998
16000	.99818	.00128	.00049	.99995

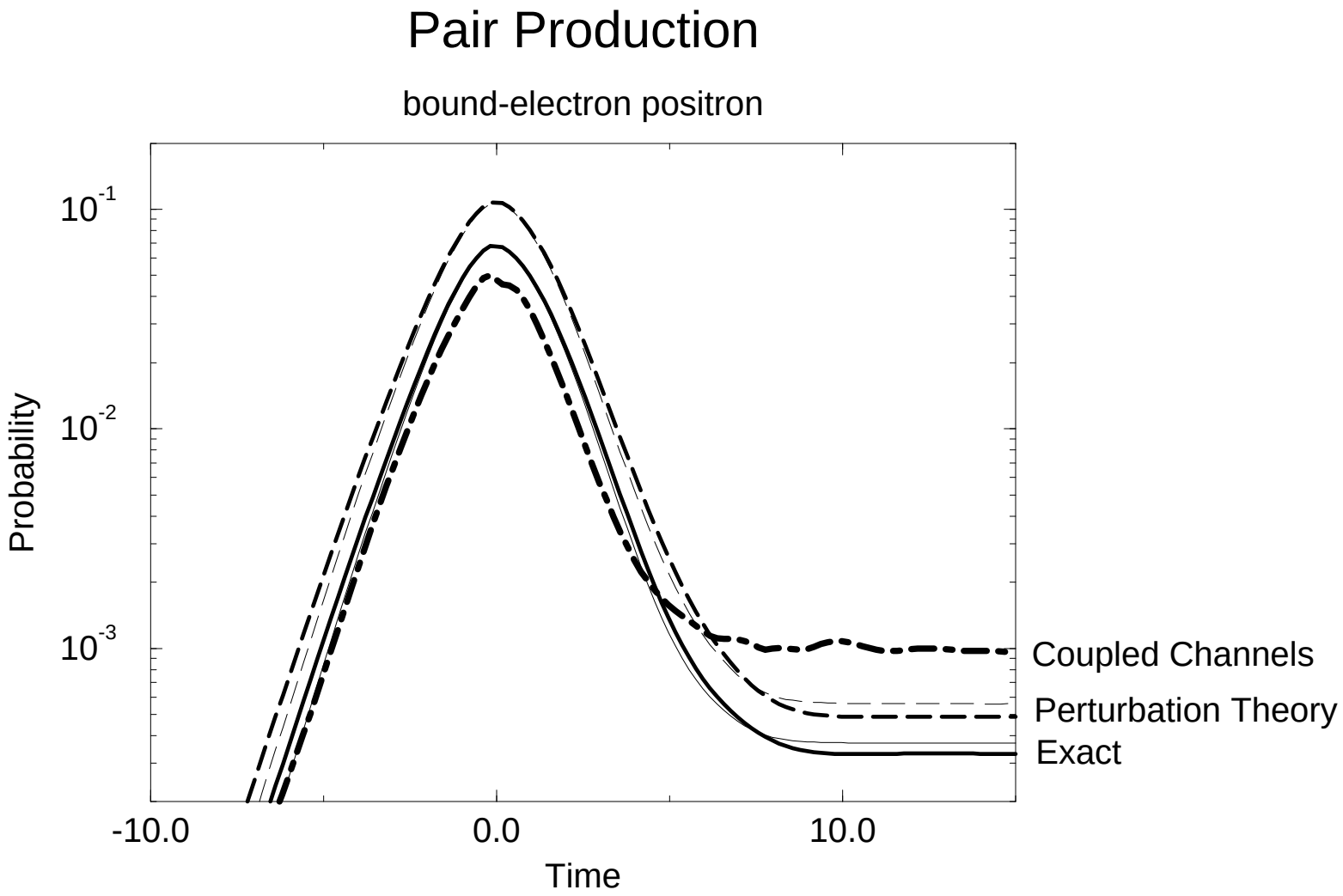
Pair Production
bound-electron positron
Probability
10^{-1}
10^{-2}
10^{-3}
-10.0
0.0
10.0
Time
Coupled Channels
Perturbation Theory
Exact

Fig. 1